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MODELING FREEZING PROCESSES WITH THE FINITE POINTSET METHOD

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Abstract. We present an approach to model the process of freezing and melting of fluids including expansion of volume with the Finite Pointset Method (FPM). The model is based on defining a freezing range of temperatures in which phase transition occurs and letting the material parameters of the freezing fluid (density, thermal conductivity, specific heat capacity) depend on temperature. Also coupling to other materials which is necessary for damage prediction is discussed.

1 INTRODUCTION

We are concerned with the modeling problems involving damages in containers by freezing fluids. If for example a water filled pipe is exposed to low temperatures, the water in the pipe can freeze. Since this goes along with volume expansion of the fluid the pressure within the pipe will increase. If the pressure is too high damages at the pipe can be caused.

There is a lot of applications which involve freezing processes for example in civil engineering where aritficial ground freezing is used in tunnel construction or in food sciences for the preservation of fresh food. The main task is to estimate the time until the piece of food or the ground is fully frozen. Most of modeling approaches for these kind of problems do not consider the change of volume of the fluid when freezing. Often only a temperature equation with temperature dependent parameters is used.

However, we want to focus on applications where the change of volume is an essential part of the freezing problem, for example in the evaluation whether a closed pipe will withstand high pressures due to expanding freezing fluid, or, if there is a system of pipes, in the determination of the freezing order.

We model the freezing liquid over the Navier Stokes Equations with temperature dependent material parameters. The expansion of ice is included into the modeling process by a temperature and pressure dependent density.

For the numerical realization particle methods are preferred on mesh-based for including the expansion of volume of the fluid because in meshless methods there are no restrictions for the deformation of the grid. Advantageous for this kind of problems is also the possibilitiy of dealing with free surfaces. Our implementation of the model is done with the Finite Pointset Method (FPM), a method (and code) for performing fluid and continuum mechanical simulations developed at the Fraunhofer Institute for Industrial Mathematics (ITWM), [5]. FPM is a generalized finite difference method using a cloud of numerical points as data carriers. It establishes approximations of derivatives by a specialized least square algorithm.

We illustrate the model on a simple example — the freezing of a pipe.

2 MODELING OF FREEZING PROCESSES

We model the liquid and the solid phase of the fluid as a single material with material properties being temperature dependent. For modeling the fluid flow we use the Navier Stokes equations in Lagrangian form consisting of the conservation laws for mass and momentum

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho(\nabla \cdot \mathbf{v}) = 0 \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho\mathbf{v}) + (\rho\mathbf{v}) \cdot (\nabla \cdot \mathbf{v}) = -\nabla p + \rho \cdot \mathbf{g} + \nabla \cdot \mathbf{S}^{\mathrm{T}} \tag{2}$$

where the unknowns are the velocity $\mathbf{v}$, the momentum $(\rho\mathbf{v})$ and the pressure p. Moreover, $\rho = \rho(T, p)$ denotes the pressure and temperature dependent density, $\mathbf{g}$ the body forces and

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \tag{3}$$

the material derivative. The stress tensor $\mathbf{S}$ composes of a solid and a viscous part $\mathbf{S} = \mathbf{S}_{\text{viscous}} + \mathbf{S}_{\text{solid}}$ with

$$\mathbf{S}_{\text{viscous}} = \eta\frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{dt}} \qquad \text{and} \qquad \frac{\mathrm{d}\mathbf{S}_{\text{solid}}}{\mathrm{d}t} = \mu\frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{d}t} + \mathbf{K} \cdot \mathbf{S}_{\text{solid}} - \mathbf{S}_{\text{solid}} \cdot \mathbf{K} \tag{4}$$

where the strain rate tensor is given by

$$\frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{d}t} = \left[\frac{1}{2}\left(\nabla\mathbf{v}^{\mathrm{T}} + \left(\nabla\mathbf{v}^{\mathrm{T}}\right)^{\mathrm{T}}\right) - \frac{1}{3}(\nabla^{T} \cdot \mathbf{v}) \cdot \mathbf{I}\right] \tag{5}$$

and $\mathbf{K} = \frac{1}{2}\left(\nabla\mathbf{v}^{\mathrm{T}} + \left(\nabla\mathbf{v}^{\mathrm{T}}\right)^{\mathrm{T}}\right)$ is due to the the rigid rotation. The dynamic viscosity is denoted by $\eta = \eta(T)$ and the modulus of elasticity by $\mu = \mu(T)$ (linear elastic, Hook model). Both are temperature dependent because we want to capture the different properties of solid and liquid phase temperature dependent in one material, e.g. the modulus of elasticity will vanish for the liquid state and be very large in the solid state.

The temperature T is modeled over the conservation law of energy

$$(\rho C_v)\frac{\mathrm{d}}{\mathrm{d}t}T = \nabla\cdot(\mathbf{S}\cdot\mathbf{v}) - (\nabla\cdot\mathbf{S})\cdot\mathbf{v} - \mathrm{p}\nabla\cdot\mathbf{v} + \nabla\cdot(\kappa\nabla\mathrm{T}) \tag{6}$$

where the (temperature dependent) constants are the thermal conductivity $\kappa = \kappa(T)$ and the specific heat capacity $C_v = C_v(T)$. Heating due to local dissipation is included on the right hand side via the terms $\nabla\cdot(\mathbf{S}\cdot\mathbf{v}) - (\nabla\cdot\mathbf{S})\cdot\mathbf{v}$, heating due to local compression by $-p\nabla\cdot\mathbf{v}$ and heating due to heat conduction in $\nabla\cdot(\kappa\nabla T)$.

Note that an incompressible approach would not be valid as the density will vary much with temperature when the fluid goes through a phase change.

2.1 Freezing range

Depending on the fluid considered there is not only a freezing point where the liquid phase immediately turns into solid phase when being further cooled down. For some fluids there is a freezing range of temperatures where the liquid phase first turns into a transition phase. When further being cooled down and leaving this temperature range again then this transition phase of the fluid turns solid. Especially if the fluid is a mixture of other fluids with different freezing points. First, the liquid with highest freezing point turns solid and the whole fluid goes to a transition state. The whole mixture turns solid as soon as the temperature drops below the lowest freezing point.

It follows that there are three temperature regimes which typically have to be considered. Let $T_L \geq T_H$ be temperatures such that below a temperature T_L there is the solid regime, above T_H there is the liquid phase and the blending range $[T_L, T_H]$. In the case where $T_L = T_H$ there is no blending regime, but only a freezing point.

2.2 Material properties in liquid state

We will now specify the material properties in liquid state, that is for temperatures above the freezing range $T \geq T_H$. In application with freezing very high pressures can occur yielding a compression of the liquid. The equation of state relating the liquid density ρ of hardly compressible fluids to pressures p is the well-known Tait equation

$$p - p_{liq,0} = B\left(\left(\frac{\rho}{\rho_{liq,0}}\right)^m - 1\right) \tag{7}$$

where $p_{liq,0}$ and $\rho_{liq,0}$ are reference values for pressure and density, respectively. The constants B and m (the heat capacity ratio) are given by the relation

$$B = \frac{\rho_{liq,0}c_0^2}{m} \qquad \text{and} \qquad m = \frac{C_p}{C_v}, \tag{8}$$

where c_0 is the speed of sound, C_p the heat capacity at constant pressure and C_v the heat capacity per volume.

2.3 Material properties of solid state

We will now specify the material properties in solid state, that is for temperatures below the freezing range $T \leq T_L$. Our material model for the solid phase considers two aspects. Firstly, water ice is well known to further expand when freezing. Secondly, ice can be compressible because it is not a homogeneous medium and might contain air bubbles. We model the density of ice ρ_{Ice} as

$$\rho_{Ice}(T, p) = \rho_{Ice,0} + c_p p \tag{9}$$

where $\rho_{Ice,0}$ is a reference density at $T = T_L$ and no pressure applied. The non-negative constant c_p is a compressibility constant. If it is positive the fluid increase its density for increasing pressures. In the case of water the parameters can be set to $\rho_{Ice,0} = 911.0\text{kg/m}^3$, and $c_p = 10^{-10} \dots 10^{-6}$.

2.4 Blending liquid and solid phase

In the blending phase where the temperatures lie in the range $[T_L, T_H]$ the state transition from solid to liquid and vice versa needs to be modeled. For the heat transfer coefficient κ, the density ρ, the dynamic viscosity η and the shear modulus μ we specify a linear blending, so the density is given by Equations (7) and by (9) in the liquid and solid phase, respectively.

$$\rho(T, p) = \begin{cases} \rho_{Ice}(T, p) & \text{if} \quad T < T_L \\ \sqrt[m]{\frac{p - p_{liq,0}}{B} + 1} & \text{if} \quad T > T_H \\ \text{linear blend} & \text{if} \quad T_L \leq T \leq T_H \end{cases} \tag{10}$$

In the blending for the specific heat capacity C_v we need to take care of the latent heat L_h which is the heat released or absorbed during a process that occurs without a change in temperature - here during phase transition. The blending needs to be modeled such that

$$\int_{T_L}^{T_H} C_v(T) \mathrm{d}T = L_h \tag{11}$$

is fulfilled. This can be done in several ways, we stick to $C_v(T) = \frac{L_h}{(T_H - T_L)}$. In order to have this condition well-defined we always assume $T_H > T_L$, so even for fluids which have a determined freezing point a small freezing interval is assumed.

2.5 Water data

Though water is known to have a single freezing point we assume to have a freezing range between $T_L = 272$ K and $T_H = 274$ K to include the latent heat. The material parameter of water are found in Tables 1–2.

Figure 1: Temperature dependent specific heat capacity of water.

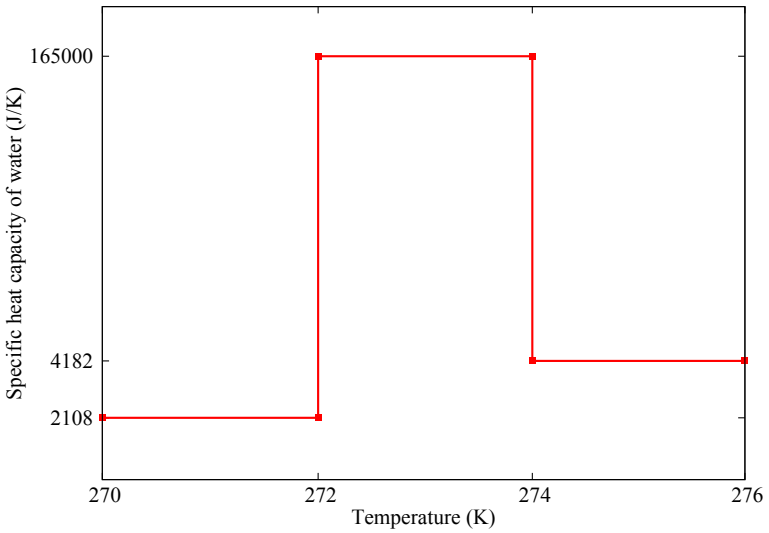


Table 1: Material parameters for water: density model, Equation (10).

Parameter	Value	Meaning
$\rho_{liq,0}$	1000.0 kg/m^3	reference density liquid phase
$p_{liq,0}$	0 Pa	reference pressure liquid phase
B	0.3214 GPa	
m	7	heat capacity ratio
$\rho_{ice,0}$	911.0 kg/m^3	reference density solid phase
c_p	10^{-8} s^2/m^4	compressibility constant

Table 2: Material parameters for water.

Parameter	$T \geq T_H$ (liquid)	$T \leq T_L$ (solid)	$T_L < T < T_H$ (blending)
κ	2 W/(m K)	0.5 W/(m K)	linear
C_v	4182 J/kg K	2108 J/kg K	$L_h = 333000$ J/kg
μ	0 Pa	$1e9$ Pa	linear

2.6 Temperature-only example

A first numerical example is given to demonstrate the behaviour of temperature only in a cooling scenario. We assume zero velocity and pressure at all times, and solve only Equation (6) for the temperature with temperature varying density, specific heat capacity and heat conductivity.

Let there be a fluid domain geometry Ω (here it is a cylinder) with boundary $\partial\Omega$ and outward normal $\mathbf{n}$. Initially the water shall be of constant temperature (300K). At the boundary of the fluid domain we apply a convective boundary condition

$$\alpha(T - T_{out}) + \kappa \nabla T \cdot \mathbf{n} = 0 \tag{12}$$

where T_{out} is the outside temperature (here 250 K) and α is the heat transfer coefficient (here $50\mathrm{W/m^2\,K}$).
For a point within the domain the temperature is typical of the form as in Figure 2. In the beginning there is a rapid decay from the initial temperature to the upper limit of the freezing range. In the freezing range the cool down is slowed down due to the high heat capacity. After leaving the freezing range again, the cool down speeds up and asymptotically reaches the outside temperature T_{out}. The cooling rate depends on the heat transfer coefficient α and the surface area of the fluid domain.

3 REALIZATION OF FULL MODEL IN FPM

Let the fluid domain be discretized with an initial particle configuration. Each particle shall have an initial temperature, velocity and pressure, we denote the initial state of the system by (T_0, v_0, p_0). Assume also that appropriate boundary conditions are given.

In each timestep (i) corresponding to a time t_i we first compute the new temperature T_i from Equation (6) on all particles due to the temperature boundary conditions and parameters depending on (T_{i-1}, p_{i-1}), which are

$$\kappa = \kappa(T_{i-1}), C_v = C_v(T_{i-1}) \text{ and } \rho = \rho(T_{i-1}, p_{i-1}). \tag{13}$$

With the new temperature T_i we update the temperature dependent material properties of the fluid $\rho(T_i, p_{i-1}), \eta(T_i)$ and $\mu(T_i)$ for each particle. Then we solve the Navier Stokes equations (2) for velocity and pressure discretized in an implicite scheme. Having now computed the velocity, particles are moved with this velocity field. An adaption of the pointcloud is done in order to preserve a good quality pointcloud, [5].

4 COUPLING CONDITIONS

In order to be able to consider settings which involve coupling of the freezing fluid to other materials also appropriate coupling conditions have to be specified. Assume there are two materials having contact, where material properties f are denoted by subscripts f_L for one material and by f_R for the other. The contact surface shall have normals $\mathbf{n}_\mathrm{L} = -\mathbf{n}_\mathrm{R}$ and the tangential space shall be spanned by $\mathbf{t}_1$ and $\mathbf{t}_2$.

The conditions for the temperature are the continuity of the heat fluxes $\kappa\nabla T \cdot \mathbf{n}$ over the contact surface and a heat transfer condition with heat transfer coefficient α

$$\kappa_L \nabla T_L \cdot \mathbf{n}_\mathrm{L} + \kappa_\mathrm{R} \nabla \mathrm{T}_\mathrm{R} \cdot \mathbf{n}_\mathrm{R} = 0 \qquad \text{and} \qquad \alpha(T_R - T_L) + \kappa_R \nabla T_R \cdot \mathbf{n}_\mathrm{R} = 0. \tag{14}$$

For velocity $\mathbf{v}$ and pressure p we have the following conditions. Due to equilibrium of tension at the contact surface the tangential tensions of both sides must coincide. The velocity is divergence free in the contact surface and the normal tensions balance. This yields four conditions

$$\mathbf{t}_\mathrm{i}^\mathrm{T} \mathbf{S}_\mathrm{L} \mathbf{n}_\mathrm{L} = \mathbf{t}_\mathrm{i}^\mathrm{T} \mathbf{S}_\mathrm{R} \mathbf{n}_\mathrm{R}, \mathrm{i} = 1, 2, \qquad \mathrm{div}(\mathbf{v}_\mathrm{L}) = 0, \qquad \mathbf{n}_\mathrm{L}^\mathrm{T} \mathbf{S}_\mathrm{L} \mathbf{n}_\mathrm{L} - \mathrm{p}_\mathrm{L} = \mathbf{n}_\mathrm{R}^\mathrm{T} \mathbf{S}_\mathrm{R} \mathbf{n}_\mathrm{R} - \mathrm{p}_\mathrm{R}. \tag{15}$$

Moreover the normal velocities shall coincide, the tangential forces shall underly a slip condition with slip coefficient β and a condition relating the pressure gradients on both sides are assumed — yielding four more conditions

$$\mathbf{v}_\mathrm{R}^\mathrm{T} \mathbf{n}_\mathrm{R} = \mathbf{v}_\mathrm{L}^\mathrm{T} \mathbf{n}_\mathrm{L}, \qquad \mathbf{n}_\mathrm{R}^\mathrm{T} \frac{1}{\rho_\mathrm{R}} \nabla \mathrm{p}_\mathrm{R} = -\mathbf{n}_\mathrm{R}^\mathrm{T} \frac{1}{\rho_\mathrm{L}} \nabla \mathrm{p}_\mathrm{L} \tag{16}$$

$$\mathbf{t}_\mathrm{i}^\mathrm{T} \mathbf{S}_\mathrm{R} \mathbf{n}_\mathrm{R} + \beta(\mathbf{v}_\mathrm{R} - \mathbf{v}_\mathrm{L})^\mathrm{T} \mathbf{n}_\mathrm{R} = 0, \mathrm{i} = 1, 2. \tag{17}$$

5 NUMERICAL EXAMPLE

5.1 Setting

We demonstrate the modeling of freezing processes on a simple example. The geometry is part of a water filled pipe, which is a cylindrical container filled with water with inner radius 9 mm, outer radius 10 mm and length 50 mm, see Figure 3.

Both ends are kept fixed fixed during the simulation. Initially we assume there is zero velocity and pressure everywhere and constant temperature 274.15 K which is above the transition interval.

In the setting there is cooling from outside over the container (assumed outside temperature 250K and heat transfer coefficient $50\mathrm{W/m^2}$). Over the contact of container material and fluid we set a heat transfer coefficient of $300\mathrm{W/m^2\,s}$. The fluid will cool then and expand as it freezes.

There will be forces arising in the fluid pushing against the container material where we use a Johnson–Cook material model, [2, 4] giving a relation between equivalent stress and equivalent strain

$$\mathbf{S}_\mathrm{JC} = (\mathrm{A} + \mathrm{B}\varepsilon_\mathrm{p}^\mathrm{n}) \cdot (1 + \mathrm{C} \log\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)) \cdot (1 - \mathrm{T}_\mathrm{hom}^\mathrm{m}). \tag{18}$$

The parameters are the yield stress A, B and n are related to the plastic flow, C is a parameter for the sensitivity of the strain rate in the second term. The plastic strain

ε_p measures the deformation after reaching the yield stress and the plastic strain rate is $\dot{\varepsilon_p} = \frac{\dot{\varepsilon}}{\dot{\varepsilon_0}}$. The temperature T_{hom} is defined as

$$T_{hom} = \frac{T - T_0}{T_m - T_0} \tag{19}$$

where T_0 is a reference temperature and T_m is the melt temperature. Here $T_{hom} \approx 0$ is assumed because the setting is far away from the regime of melting temperatures of the container material.

For the testing of our numerical approach we choose a container material which has a low yield stress. The parameters are given in Table 4.

5.2 Results

The temperature of container decreases quite fast and there is a good heat transfer to the fluid in the inner, see Figure 4. The temperature of the water stays in the transition interval until approximately 1850 seconds (shortly after the fifth image) and quickly drops after leaving the transition interval. The expansion of the fluid with temperature yields also stresses onto the container material, which cause first elastic deformations and if the stresses are high enough also plastic deformations, see Figures 5 and 6.

6 FUTURE WORK

We presented a model for simulating the expansion of fluids when freezing with coupling to other materials where the phase transition is modeled over a transition interval in temperature. Future investigations should try to reduce this interval in the case of water. Also the parameters for the compressibility of ice are not clear, but they are very important because they influence the pressures and stresses. Further investigations should be done there as well.

Figure 2: Typical temperature behaviour in the freezing model.

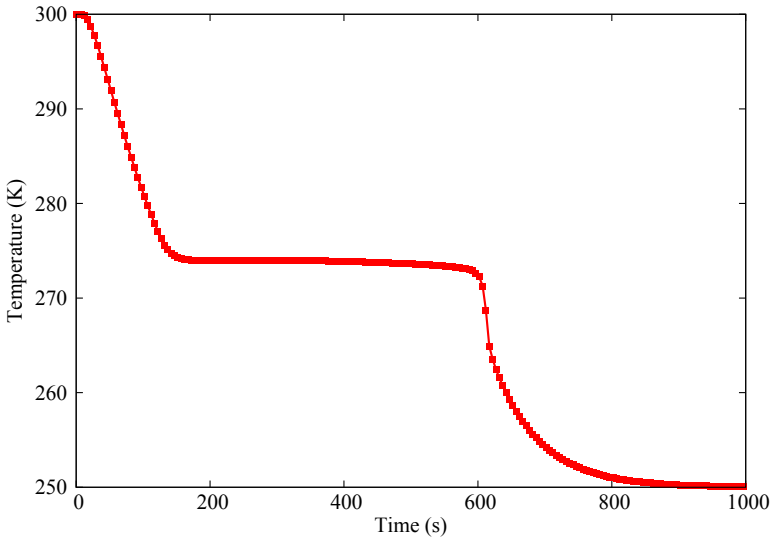


Figure 3: Geometry of simple illustrating example: red showing the chamber of the container material, blue showing the chamber of water.

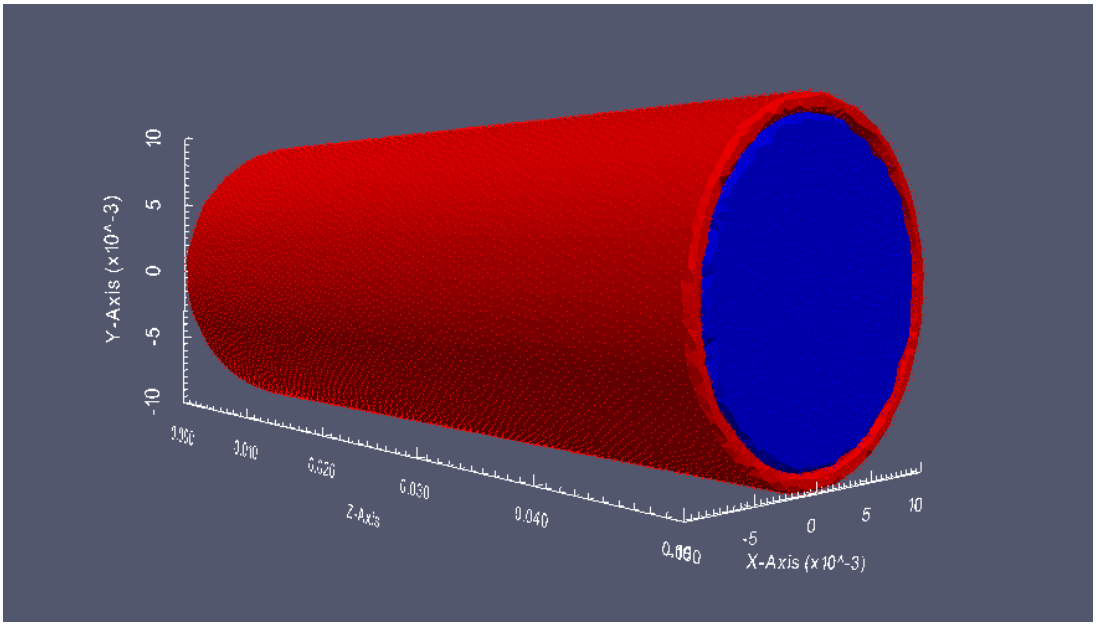


Figure 4: Snapshots of temperatures in slice of the pipe.

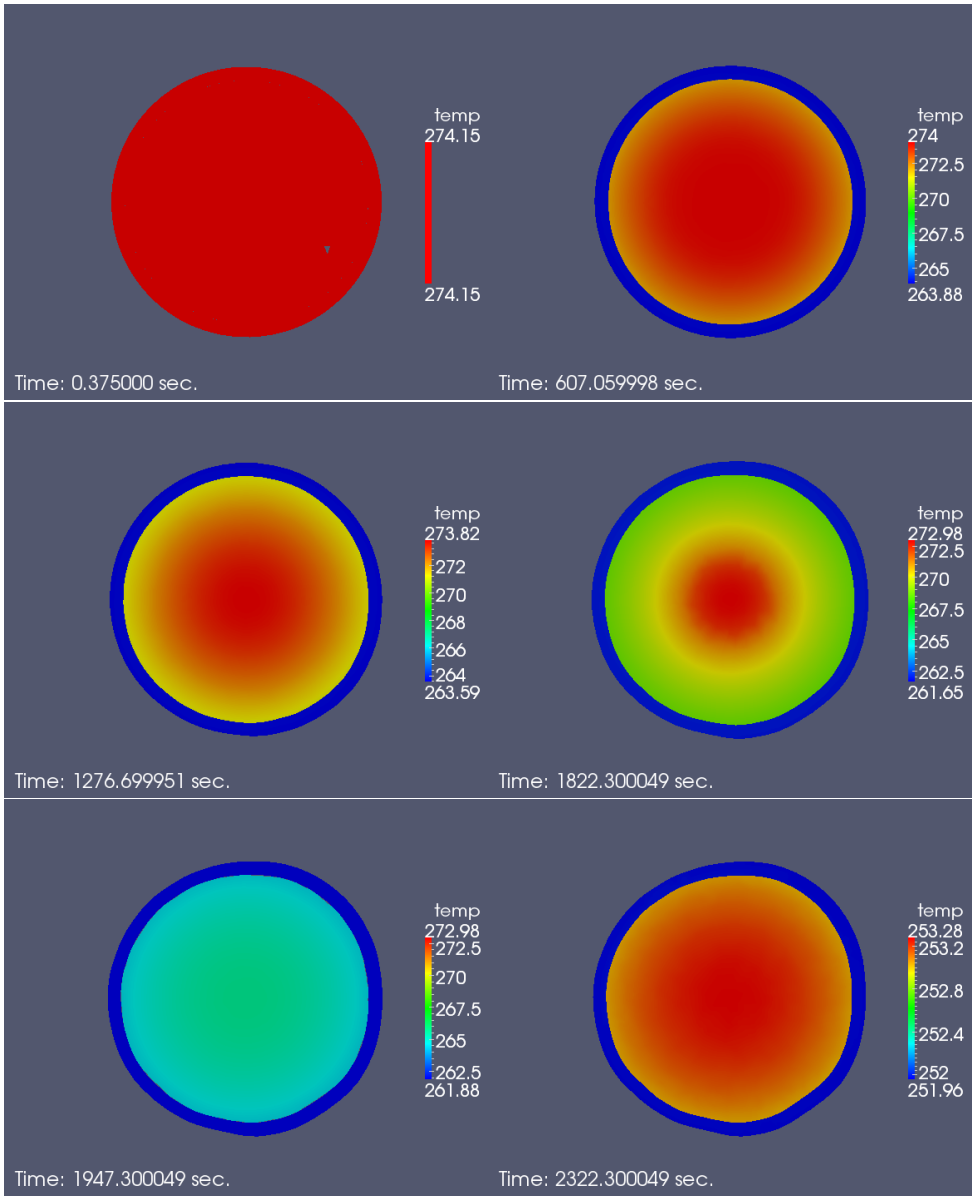


Table 3: Material parameters for Johnson–Cook model for the container material.

Parameter	A	B	C	ε_0	n
Value	510e2 Pa	1e5	1.0	0.65	0.07

Table 4: Other parameters for container material.

Parameter	ρ	κ	C_v	μ
Value	2000 kg/m^3	10.0 W/m K	440 J/kg K	7690000 Pa

Figure 5: Pipe: undeformed state at the beginning of freezing, final state fully cooled down.

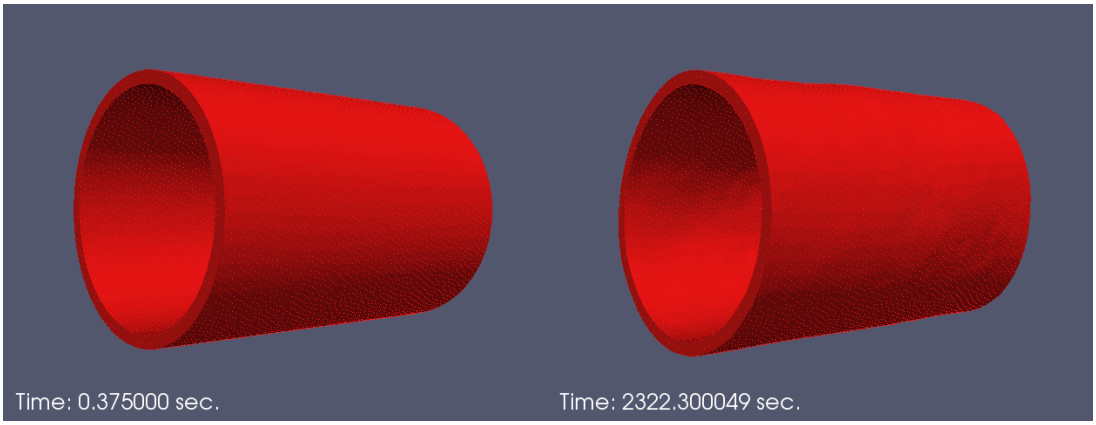
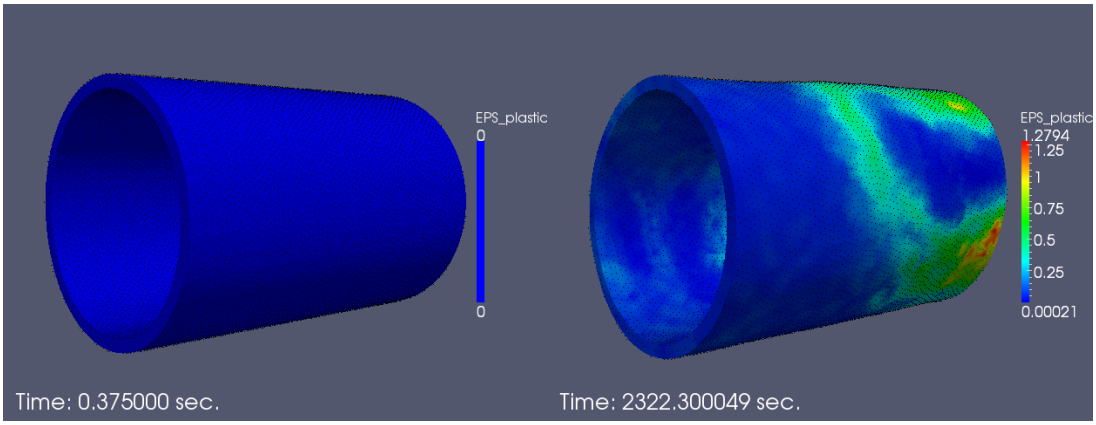


Figure 6: Pipe: plastic deformation.



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